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Ground state energy in a spherical GaAs-(Al,Ga)As quantum dot with parabolic confinement

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bstract : An attempt is made to derive the ground state energy of a spherical dot having finite quantum well with parabolic potential The rived result is computed as a function of the size of GaAs-Al$_x$Ga$_{1-x}$As spherical quantum dot, for different barrier heights of the potential well The ound level in a parabolic dot is found to lie much higher than that in a similar dot with square-well potential.

eywords Quantum dot, energy levels, semiconductors, III-V compounds

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Introduction

uantum dots (QDs) are designable mesoscopic atoms easily tegrable in bulk electronics. Such zero-dimensional structures, ing solid state systems with an atomic like density of states, ve attracted much interests for an efficient replacement of her quantum heterostructures for emerging semiconductor vices. These semiconductor QDs exhibit various interesting operties, which indicate their large applicability to electronic d optoelectronic devices [1-5]. For designing and proper nctioning of these devices, the quantized energy level uctures in such quasi-zero dimensional (QOD) systems have be known very accurately.

Studies reported on QOD structures have mostly dealt with uantum wells (QWs) having square well potential (SWP) with nite or infinite barrier height. But in practically realizable QWs, e potential profiles assume a parabolic form rather than the uare or rectangular shape, which has been so prevalent. ecently, few works on parabolic well with infinite barrier height ave been reported [6,7]. But considering a well with a finite arrier height is a more practical approach, since potential well ith infinite barrier height is not realizable at all. The most popular air of lattice-matched materials used for the realization of a heterostructure is GaAs and Al$_x$Ga$_{1-x}$As. At the heterointerface of these two materials, the maximum conduction band edge discontinuity which acts as the well barrier is limited to only 0.33eV. Thus, the actual scenario is far from the ideal case for an infinite barrier QW, and the finiteness of the well barrier must be taken into consideration in order to estimate the electronic energy states in a QD.

In this communication, the lowest electronic state will be derived for a finite barrier spherical QD with parabolic confinement. The ground level energy will be computed for GaAs - Al$_x$Ga$_{1-x}$As QDs of different barrier heights realized by varying Al-concentration (x) in (Al,Ga)As alloy, the barrier material.

2. Theoretical background

The Hamiltonian in a spherical QD can be expressed, in the effective mass approximation, as

$$H_0 = -\left(\hbar^2/2m^*\right)\nabla^2 + V(r), \tag{1}$$

where m^* is the effective mass of electron. For a dot of radius R with parabolic potential well, the confining potential $V(r)$ can be described as

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$$V(r) = \begin{cases} (1/2)m_w^* \omega^2 r^2, & r \le R, \\ V_0, & r \ge R, \end{cases} \tag{2}$$

where m_w^* is the effective mass of electron in the dot material, ω is the parabola frequency, and V_0 is the height of the potential barrier. In a finite QD, V_0 is essentially the conduction band offset due to the band gap discontinuity between GaAs, the dot material and $Al_xGa_{1-x}As$, the embedding material. In the case of a parabolic QD, the barrier height is related to the dot size through the relation

$$V_0 = (1/2)m_\omega^* \omega^2 R^2. \tag{3}$$

Using the above conditions, the Schrödinger equation for the well and the barrier regions can be written as:

$$-\left(\hbar^2/2m_\omega^*\right)\nabla^2\psi + (1/2)m_\omega^*\omega^2 r^2 \psi = E\psi,$$

$$\text{for} \quad r \le R \tag{4a}$$

and

$$-\left(\hbar^2/2m_b^*\right)\nabla^2\psi + \nabla_0 \psi = E\psi,$$

$$\text{for} \quad r \ge R, \tag{4b}$$

where m_b^* is the effective mass of electron in the barrier material.

For a spherical QD, the electron wavefunction corresponding to the unperturbed Hamiltonian can be written in the standard factorized form [8] as

$$\psi(r, \theta, \phi) = \frac{1}{r}\, \chi_l(r)\, Y_{lm}(\theta, \phi), \tag{5}$$

where $\chi_l(r)$ and $Y_{lm}(\theta,\phi)$ are the radial and the angle dependent parts of the wavefunction; l, m being the associated quantum numbers.

The above factorization yields the radial part of eq.(4a) as

$$d^2\chi_l(r)/dr^2 + \left[k^2 - \lambda^2 r^2 - l(l+1)/r^2\right]\chi_l(r) = 0, \tag{6}$$

where $k^2 = 2m_\omega^* E/\hbar^2$ and $\lambda = m_\omega^* E/\hbar$.

The solution to this equation is of the form [8]

$$\chi_l(r) = C\, r^{l+1} Exp\left(-\lambda r^2/2\right)$$

$$U\left[(l+3/2-\mu)/2, (l+3/2); \lambda r^2\right], \tag{7}$$

where U stands for confluent hypergeometric function, C is a constant and $\mu = k^2/2\lambda = E/\hbar\omega$.

Thus, for the lowest energy level (*i.e.* $l = m = 0$), the electron wavefunction in the well region is obtained from eqs.(5) and (7) as

$$\psi_{W0} = N_1\, Exp\left(-\lambda r^2/2\right)$$

$$U\left[(3/2-\mu_0)/2, 3/2; \lambda r^2\right], \tag{8}$$

where the constant N_1 takes the value of $Y_{00}(\theta,\phi)$ and the constant C into account, and $\mu_0 = E_0/\hbar\omega$, E_0 being the ground state energy of the QD.

For calculations pertaining to the barrier, the ground state wave function ψ_{b0} can be obtained in a similar manner, as

$$\psi_{b0} = N_2 (1/r)\, Exp(-\chi_0 r), \tag{9}$$

where $\chi_0 = \left[2m_b^*(V_0 - E_0)/\hbar^2\right]^{1/2}$ and N_2 is another constant to be determined from the continuity of the wave function at the well boundary. The electron wavefunction for the barrier region ψ_{b0} thus finally becomes

$$\psi_{b0} = N_1 R\, Exp\left(-\lambda R^2/2\right)$$

$$U\left[(3/2-\mu_0)/2, 3/2; \lambda R^2\right](1/r)\, Exp\left[\chi_0(R-r)\right] \tag{10}$$

Further application of the boundary condition for current continuity across the interface between the dot and the embedding material, yields the following transcendental equation

$$\frac{2U^1\left[(3/2-\mu_0)/2, 3/2; \lambda R^2\right]}{U\left[(3/2-\mu_0)/2, 3/2; \lambda R^2\right]} = 1 - \frac{m_\omega^*}{\lambda m_b^*}\left[(\chi_0 + 1/R)/R\right], \tag{11}$$

where U^1 is the derivative of the confluent hypergeometric function U with respect to λr^2. Solving the above eq.(11) numerically, the lowest unperturbed energy E_0 of an electron confined in a spherical QD with finite barrier parabolic potential well can be obtained.

3. Discussion

For numerical computation of the ground state energy in a finite GaAs-$Al_xGa_{1-x}As$ QD, we have assumed that the band gap discontinuity in these two semiconductors is distributed about 60% on the conduction band and 40% on the valence band, while the total band gap difference is a function of Al-concentration (x) given by ΔE_g (eV) = $1.247\,x$.

Here, all the material parameters of GaAs and $Al_xGa_{1-x}As$ have been taken from Ref. [9]. In the present analysis, the value of Al-concentration has been limited to 0.45, since for higher x the nature of energy band structure of the $Al_xGa_{1-x}As$ alloy changes to indirect band gap, and the present barrier height treatment will no longer be valid. Figure 1 exhibits the variation he ground state energy with the radius of a spherical GaAs-$Al_xGa_{1-x}As$ QD with parabolic potential well, for three different alloy compositions. The obvious lowering in the ground level energy with increase in dot size is evident from the figure; lack of carrier confinement in large dots being responsible for such energy lowering. For the sake of comparison, standard established results for spherical GaAs-$Al_xGa_{1-x}As$ QD with SWP have also been presented in the same figure.

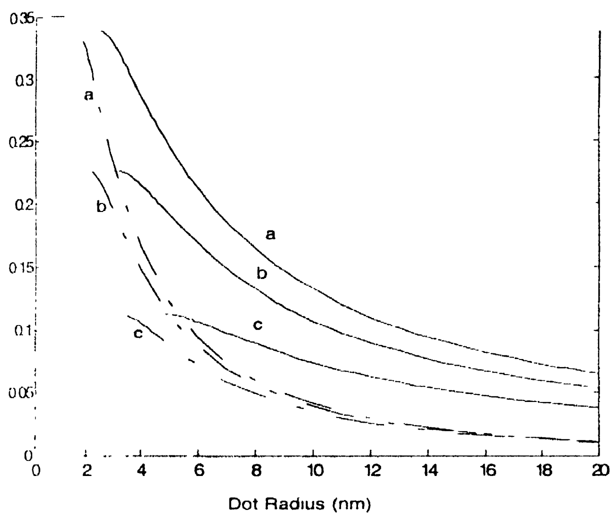

Figure 1. The ground state energy as a function of the radius R of a spherical GaAs-$Al_xGa_{1-x}As$ QD with a parabolic (solid) and a square (broken) well potential for three different Al concentrations: (a) $x = 0.45$, (b) $x = 0.30$ and (c) $x = 0.15$

A comparison between the energy levels in a QD with parabolic and square well potential leads to the conclusion that the physical confinement of the carrier is stronger in the case of parabolic potential. In the case of a square well, throughout its height, the width of the well is uniform and equal to the dot diameter $2R$. But, in the case of a parabolic well, the well width varies within the dot; starting from zero at the bottom of the well, its width increases gradually to the maximum value $2R$ at the top of the well where the barrier height is V_0. Therefore, carriers in a parabolic well can be thought of as being confined in an effectively smaller dot with respect to those in a square well. As a result, the carrier confinement is stronger in a QD with parabolic potential profile and the lowest energy level lies higher than the corresponding energy level in a dot with SWP. It is further to be noted that in the case of SWP, the ground levels for QDs with different barrier heights converge for large dots. The energy level then approaches to that in bulk material, where the carrier confinement is so weak that even a small increase in the height of the potential barrier V_0 will not cause any appreciable shift in the corresponding energy levels. On the other hand, in the case of a QD with parabolic potential well, the radius of a quite large dot is effectively small at the bottom of the QW, making the confinement of the carriers still feasible, and thereby maintaining distinct energy values for different barrier heights. However, in large dots, the ground state energy becomes almost independent of dot size.

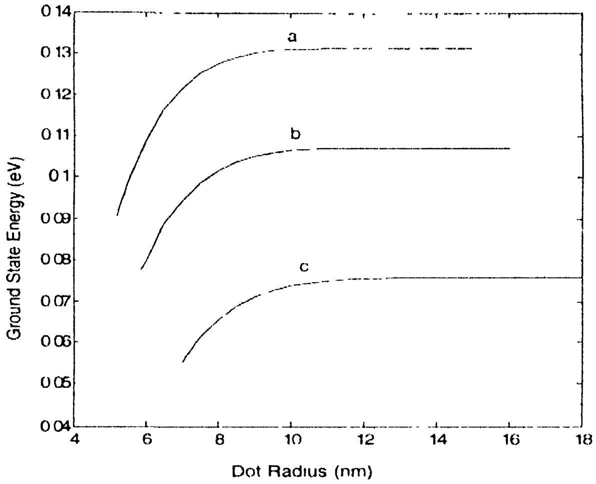

Figure 2. The ground state energy of a parabolic well as a function of the radius R of a spherical GaAs-$Al_xGa_{1-x}As$ QD for three different parabola frequencies: (a) $\omega = 3.32157 \times 10^{23}$ radian/sec, (b) $\omega = 2.71205 \times 10^{23}$ radian/sec and (c) $\omega = 1.91771 \times 10^{23}$ radian/sec

Figure 2 shows the variation of the ground state energy with the dot radius for different curvatures of the confining parabolic potential. Here, the typical values of curvature for the parabolic potential *i.e.*, those of parabola frequency ω have been estimated from eq.(3) for a dot of radius 10 nm, with three barrier heights V_0 corresponding to three Al- concentrations x = 0.45, 0.30 and 0.15. The figure shows that as the dot radius goes on increasing, the ground level energy initially increases and gradually saturates. For a finite potential well, the barrier height is related to the dot radius through eq.(3). Therefore, for a particular value of ω, the barrier height V_0 essentially increases with dot size, resulting in stronger carrier confinement and thereby, lifting the lowest energy level. However, such effect is prominent only upto moderately large dots. Beyond those values of dot radii, the carrier confinement becomes so weak due to the size of the quantum dot itself that further increase in V_0 does not influence the ground energy significantly. Thus, the energy levels for different ω eventually saturate with increasing dot radius; smaller the value of ω, larger the value of dot radius at which the energy saturation takes place.

4. Conclusion

In the present work, the ground state energy in a spherical QD having finite quantum well with parabolic potential has been derived. The derived result has been computed as a function of the dot size for different barrier heights of the potential well formed in a GaAs – (Al,Ga)As QD. In a finite QD, higher values of ground level energy have been obtained in a well with parabolic potential as compared to that of SWP. Therefore, our observation implies a stronger confinement in a practically realizable QD, where the confining potential can be better described by a parabola rather than a square - the most common and simple assumption.

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